Book Review

Modern Electronic Structure Theory. *Edited by David R. Yarkony, World Scientific Publishing Co. Pte. Ltd., 1995, Part I, 768 pp., $152 cloth / $89 paperback, Part II, 784 pp., $152 cloth / $89 paperback*

This monograph is a collection of 22 independently written chapters on various aspects of electronic structure theory. The intent of the book is to describe from a practical perspective the present state of electronic structure theory. Several of the chapters are written at a level suitable for advanced graduate students aspiring to become developers of new programs and methods, while other chapters summarize recent results at a level suitable to a general audience. There are method chapters devoted to multireference perturbation theory (Andersson and Roos, Hoffmann), direct methods (Almlöf), analytic derivatives (Shepard, Pulay), optimization of energies (Schlegel), Jahn–Teller effects (Dykstra), integrals (Helgaker and Taylor), coupled cluster methods (Bartlett), pseudospectral methods (Martinez and Carter), exchange-correlation functionals (Becke), and time-dependent response theory (Olsen and Jørgensen). The chapters devoted more to results cover general chemical applicability (Schaefer et al.), spin orbit effects (Heβ et al.), fullerenes (Scuseria), the H atom in a field (Silverstone), the G2 method (Raghavachari and Curtiss), astrochemistry (Kirby), transition metal complexes (Bauschlicher et al.) and electron-molecule scattering (Winstead and McKoy). These subjects cover the major method developments of the last decade. The applications, by necessity, are selective. The focus is on giving an understandable presentation of the applications with which the author is most familiar. No attempt is made to provide a comprehensive survey or review of the literature.

The advertisement for this book states that it ''provides a didactically oriented description of the latest computational techniques in electronic structure theory and their impact on several areas of chemistry. The book is aimed at first-year graduate students or college seniors considering graduate study in computational chemistry, or researchers who wish to acquire a wider knowledge of this field.'' While some of the applications chapters could possibly be read by first-year graduate students, the technique-oriented chapters are clearly aimed at more advanced graduate students interested in program development.

ERNEST R. DAVIDSON
Indiana University

J Comput Chem 18:1328, 1997

CCC 0192-8651 / 97 / 101328-01